Comparison of the experimental performance of ferroelectric CPW circuits with method of moment simulations and conformal mapping

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Experimental measurements of coplanar waveguide circuits atop thin films of ferroelectric Ba_xSr_{1-x}TiO₃ (BST) were made as a function bias from 0 to 200 V and frequency from 0.045 to 20 GHz. The resulting phase shifts are compared with method of moments electromagnetic simulations and a conformal mapping analysis to determine the dielectric constant of the BST films. Based on the correlation between the experimental and the modeled data, an analysis of the extent to which the electromagnetic simulators provide reliable values for the dielectric constant of the ferroelectric in these structures has been performed. In addition, to determine how well the modeled data compare with experimental data, the dielectric constant values were also compared to low frequency measurements of interdigitated capacitor circuits on the same films. Results of these comparisons will be presented.

Ferroelectric materials, such as Ba_xSr_{1-x}TiO₃ (BST), have nonlinear dielectric constants which can be tuned by an externally applied electric field even at temperatures above the ferroelectric phase. Because of this property, the use of ferroelectric thin films in tunable microwave components such as phase shifters, tunable filters and local oscillators, among others, has been a subject of study during the last decade.[1-4] In order to fully exploit the potential of ferroelectric thin films for optimal microwave circuits, it is necessary to have accurate measurements and modeling of the thin film ferroelectric's dielectric constant (ε_r) and its loss tangent (tanb) as a function of applied bias and frequency. Our circuit was designed as a compact, simple, probe-able, device in order to characterize films in a configuration useful as high frequency phase shifters and compare the results with other tunable structures on the same film. The experimental structure is also useful in comparing the results of different algorithms to determine the dielectric constant from the scattering (S)-parameter measurements. The ferroelectric based coplanar waveguide (CPW) structure is shown in Figure 1. The CPW's metallization consists of an adhesion layer of 15 nm chrome (Cr) followed by 1.8 µm of silver (Ag) capped with 50 nm of gold (Au). The Ba_xSr_{1-x}TiO₃ (BST) thin films with a Ba Sr cation ratios of 60:40 and 40:60 were deposited using pulsed laser ablation on MgO substrates. The BST films used in these devices have been fully described in previous publications.[1] Patterning of the CPW structure on this film was performed using standard photolithography and chemical etching techniques. The outer sections where the BST has been etched away (i.e., sections of length x in Figure 1) serve as impedance transformers in order to reduce mismatch loss.

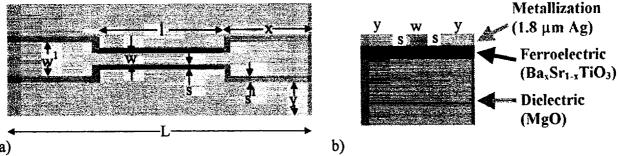


Figure 1. A ferroelectric based CPW. a.) Top-view. The inner section (of length l) contains the ferroelectric. The outer sections are 50 Ω to 30 Ω impedance transformers. This CPW has the following dimensions (in μ m): L=8000 , w¹=130 , w=100 , l=4000 , s=20 , s¹=20 , x=2000 , and y=298 . b.) Side-view of the inner section.

Using Sonnet em® [5], a commercial electromagnetic simulation software package, the CPW structure was modeled from 0.045 GHz to 20 GHz for various film dielectric constants and thicknesses. The film dielectric constant can be most easily determined by matching of the simulated and measured total transmission phase shift through the structure. The simulated phase shifts as a function of frequency for a range of dielectric constants and a BST thickness of 360 nm are shown in Figure 2(a). At any given frequency, the amount of relative phase shift increases as the dielectric constant increases. The slope of the phase shifts as a function of $\varepsilon_r(BST)$ at several film thicknesses are shown in Figure 2(b). The performance of the CPW was tested with several different applied dc voltage biases ranging from 0 V to 200 V. DC bias was

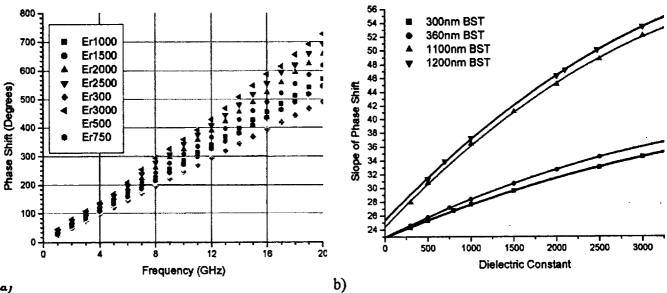


Figure 2(a). Sonnet Simulated total phase shift versus frequency for a CPW with 360 nm BST on MgO. (b) The slope of the total phase shift vs. $\varepsilon_r(BST)$ for several thicknesses.

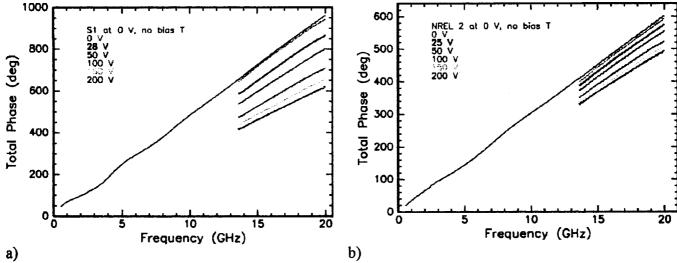


Figure 3. Total experimental phase shift versus frequency for a CPW on (a) 1200 nm and (b) 360 nm thick BST 60:40 on a MgO substrate taken at 300 K.

applied through the sample using bias tees. Since these home made high voltage bias tees operate within a limited frequency range, dc-biased data was only collected between 13.6 GHz and 20 GHz. The experimental phase shifts are shown in Figure 3. One test at 0 V without the bias tees shows the measured phase shift for frequencies down to 500 MHz.

Doubts exist as to the accuracy of the Sonnet simulations using these very high dielectric constant materials. The simple CPW circuit tested here is conducive to using this sort of planar 2D+ simulation since the dc biasing should cause the BST to tune uniformly throughout the circuit. Another analysis to which we can compare is a static conformal mapping calculation done by Carlsson and Gevorgian.[6] A comparison of data obtained using our model and that of Gevorgian is shown in Figure 4. The discrepancy between the two could arise from the fact that

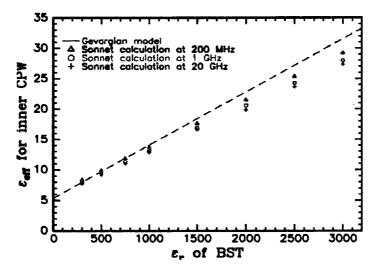


Figure 4. Comparison of our method of moments model with Gevorgian's conformal mapping method for a CPW transmission line with 360 nm of BST.

the conformal mapping does not take frequency into account (i.e., assumes zero frequency). Our software package cannot de-embed results at zero frequency, so results are shown at three different frequencies. Note that the agreement between the two models is better for frequencies below 1 GHz and for $\varepsilon_r \leq 1500$. A second method of moments electromagnetic simulator, Zeland's IE3D,[7] tested at a BST thickness of 360 nm and $\varepsilon_{r(BST)}=1000$, yielded a value of ε_{eff} on average 10% lower than the Sonnet value in a frequency range from 2 to 20 GHz.

Using the Sonnet calculations, the deconvolved ε_r of four BST thin films as a function of applied voltage is shown in Figure 5. These values were calculated using the data from 13.6 to 20 GHz (shown for 2 films in Figure 3). If one applied the conformal mapping formulas to the data, the resulting ε_r values would lie roughly 15% lower at E=0. Judging from the single BST thickness and ε_r value tested, IE3D-deconvolved values would lie approximately 10% higher than the curves in Figure 5.

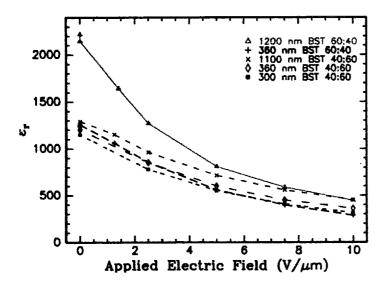


Figure 5. The dielectric constant of four BST films as determined by CPW measurements from 13.6 to 20 GHz and Sonnet em calculations.

We can also compare this method of deriving the dielectric constant to values derived from interdigital capacitor measurements. For this comparison we fabricated 50 finger interdigital capacitors with 50 fingers of length 0.69 cm with finger widths of 22 μ m and gaps of 18 μ m on the same BST films that were analyzed in Figure 5. The capacitances of these structures were measured with a HP 4192A LF Impedance Analyzer at frequencies up to 13 MHz. The capacitance was transformed to ϵ_r using another conformal analysis calculation [8] with additional corrections from Ref. [9]. Figure 6 shows a comparison of ϵ_r of 360 nm BST 60:40 film as derived from interdigital capacitor and s-parameter measurements using Sonnet. While polycrystalline low-tuning films on metallic electrodes are generally found to have frequency independent ϵ_r up to at least 20 GHz[10], higher crystalline quality high-tuning films of SrTiO₃ have been found to have ϵ_r values which drop with frequency, particularly near T_c .[11] A recent study by Booth, Vale and Ono [12] (of which we just became aware) of thin film crystalline Ba_{0.5}Sr_{0.5}TiO₃ also found ϵ_r to drop in frequency in a similar fashion. Readers should also be cautioned that the crystal orientation may be important to these ϵ_r measurements. Parallel plate structures tend to measure the dielectric constant along the polar axis, ϵ_c , while interdigital

and CPW measurements probe fields aligned to the perpendicular axis, ε_a . In thin BST films, ε_c may be significantly lower than ε_a , as is found in bulk crystalline BaTiO₃.[13] Analysis of near field microwave microscope data of BST thin films also point to this conclusion.[14]

Loss tangent analysis of our films have somewhat greater uncertainties, in part due to uncertainty in the metal conductivity, but seem to show that these films have tano values of roughly 0.02 near 1 GHz which grow to about 0.08 at 17 GHz. Application of an electric field of 10 V/µm reduces these values to about 0.005 at 1 GHz and 0.02 at 17 GHz.

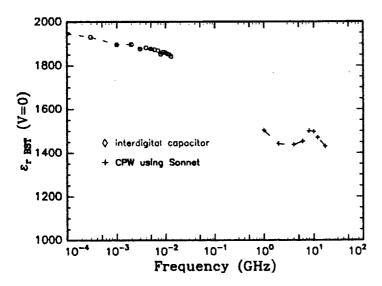


Figure 6. A comparison of ε_r of 360 nm BST 60:40 film as derived from interdigital capacitor and s-parameter measurements using Sonnet.

In conclusion, we have analyzed small probe-able CPW circuits to characterize the dielectric constant of ferroelectric thin films. We have correlated the experimental phase shifts at different applied voltage biases to the electromagnetic simulations with varying dielectric constant layers. Sonnet's em and Zeland's IE3D simulation of these CPW circuits have been found to be in reasonable agreement with low frequency interdigital capacitor measurements. Conformal mapping analyses were found to predict lower thin film BST dielectric constant values than method of moments calculations particularly at high ϵ_r (>1500) values. Discrepancies between em simulations and conformal mapping increased with frequency. A highly crystalline BST 60:40 film of thickness 1.2 μ m was found to have dielectric constants as high as 2200 and a tenability of 80% at 10 V/ μ m at frequencies up to 20 GHz.

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